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Numerical Advection Experiments With Higher Order, Accurate, Semimomentum Approximations

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ABSTRACT—Work published in 1968 by Crowley is adapted to study the truncation error associated with the semimomentum scheme for approximating advection. The results indicate that higher order approximations based on the semimomentum scheme are competitive with the best results obtained by Crowley with conservation schemes and comparable to fine-mesh calculations.

1. INTRODUCTION

This note will document a brief investigation of the use of higher order accuracy in the approximation of advection. The basic motivation for the study was to obtain a comparison between methods proposed in an earlier paper (Gerrity et al. 1972) and those studied by Crowley (1968).

Using the same analytical data as Crowley, we have made calculations with several variations of the semimomentum scheme for approximation of one-dimensional advection. The various approximations differ in theoretical accuracy. The particular data used by Crowley are characterized by local discontinuities in the first derivatives of both the initial field of the advected quantity and the advecting wind field. This fact causes some discrepancy between the theoretical properties of the finite-difference schemes and their performance in this test. Despite this logical problem, certain results were obtained that merit some notice.

2. EQUATION AND DATA

We are concerned here only with the one-dimensional calculations reported in Crowley's (1968) paper. The equation used is called the color equation. It expresses the conservation of a fluid property, ψ, following the motion of a particle; that is,

$$\frac{d}{dt}\psi=\frac{\partial\psi}{\partial t}+u\frac{\partial\psi}{\partial x}=0. \tag{1}$$

The coefficient u is the velocity of the fluid particle; in the present case, it is taken to be a function of x as follows:

$$\begin{aligned} u(x)&=0.9-1.6\ x/L \qquad 0\leq x\leq L/2,\\ u(x)&=-0.7+1.6\ x/L \qquad L/2\leq x\leq L,\\ \text{and}\qquad u(x\pm L)&=u(x). \end{aligned} \tag{2}$$

Crowley observes that, since u varies with x, one may write the nontrivial generalization of eq (1) as

$$\frac{\partial\psi}{\partial t}=-\frac{\partial}{\partial x}(\psi u)+\psi\frac{\partial u}{\partial x}. \tag{3}$$

His numerical experiments were designed to illuminate the distinction between finite-difference approximations based on eq (1), "advection schemes," and those based on eq (3), "conservation schemes." His conclusion is that a fourth-order, accurate, conservation scheme is superior to the other methods tested.

An analytic approach to the solution of eq (1) would naturally be based on the construction of the characteristic curves in the (x, t) plane. The physical meaning of the equation is that the property ψ does not vary along such curves, which one may consider to be particle trajectories.

Using eq (2) and the definition

$$\frac{dx}{dt}=u, \tag{4}$$

one may prove that the fluid particles will all repeat their relative positions, but displaced a distance L in the positive x direction, after a time interval, T, where

$$T=\frac{2L}{1.6}\ln\left[\frac{u(x=0)}{u(x=L/2)}\right]. \tag{5}$$

Thus, if one knows the distribution of ψ at some initial time and if that distribution is periodic in the x coordinate with period L, one may assert that the distribution of ψ should recur after a time lapse of T time units.

In the case studies, L=36 grid intervals of unit length. The value of the interval of repetition, T, may be given in seconds as

$$T=\frac{72}{1.6}\ln(9)=98.87. \tag{6}$$

Following Crowley, we carried out the integration through 10 such intervals, or approximately 989 s. The numerical solutions obtained at that time were compared with the analytic solution. It should be noted that the variation of u with x gives rise to a change in shape, as well as a translation, of the field ψ.

The field ψ at the initial time was set up to be

$$\psi(x)=\ln(0.9-1.6x/L) \qquad 0\leq x\leq L/2,$$
$$\psi(x)=\ln(-0.7+1.6x/L) \qquad L/2\leq x\leq L,$$

and

$$\psi(x\pm L)=\psi(x) \tag{7}$$

in agreement with Crowley's method. It should be noted that the analytical property of repetition of the solution does not depend on this specific relationship between ψ and u.

The function $\psi(x)$ defined in eq (7) has the Fourier spectrum given in table 1. During the integration, the shape of the function ψ will change; therefore, one cannot apply simple estimates of truncation error to this problem. We may note, however, that a lack of symmetry in a numerical solution may be caused by an underestimate of the "frequency" of the simulated problem, rather than by spurious dispersion.

3. THE SEMIMOMENTUM SCHEME

The basic finite-difference scheme used in this study is the semimomentum scheme introduced by Shuman (1962). Allowing Δt and Δx to stand for the time and space grid-mesh intervals, one may define symbolic, finite-difference operators. Let

$$f_j^n\equiv f(x=j\Delta x,t=n\Delta t) \tag{8}$$

where the discrete function f is defined only for integral values of the indices n and j. Our basic approximation of the first difference of the function is defined by the operator

$$[f]_x=\frac{1}{\Delta x}\,(f_{j+1/2}^n-f_{j-1/2}^n) \tag{9a}$$

or, for the time difference,

$$[f]_t=\frac{1}{\Delta t}\,(f_j^{n+1/2}-f_j^{n-1/2}). \tag{9b}$$

Since this approximation requires the use of undefined values of the function, one must couple the difference operation with an interpolation operator. A basic interpolation operator may be given the symbolic definition

$$\overline{[f]}^t=\tfrac{1}{2}(f_j^{n+1/2}+f_j^{n-1/2}) \tag{10a}$$

or, for spatial interpolation,

$$\overline{[f]}^x=\tfrac{1}{2}(f_{j+1/2}^n+f_{j-1/2}^n). \tag{10b}$$

If one uses a Taylor series expansion of the function f, one may show that these basic operations of differencing and interpolation possess second-order accuracy in the grid intervals. Thus, for functions with bounded derivatives, the error of approximation goes to zero as $(\Delta t)^2$ or $(\Delta x)^2$.

TABLE 1.—*The spectral content of the function $\psi(x)$ at the initial time. Mean value of ψ is -0.8325.*

Fourier index	Amplitude	Fourier index	Amplitude
1	0.7652	10	0.0173
2	.1846	11	.0194
3	.1444	12	.0138
4	.0677	13	.0161
5	.0634	14	.0119
6	.0363	15	.0143
7	.0370	16	.0109
8	.0236	17	.0135
9	.0254	18	.0053

The semimomentum approximation of eq (1) may be written as

$$\overline{[\psi]}_t^{\,t}=-\overline{(\overline{[u]}^x[\psi]_x)}^x. \tag{11}$$

The time derivative is a simple centered-difference approximation of second-order accuracy. The term, semimomentum, refers to the characteristic combination used to approximate the product term. Notice that the undifferentiated coefficient, the wind, is subjected to an interpolation, or a filter, prior to its multiplication by the derivative. The product is then subjected to a further interpolation, which is necessary if a staggered grid is not used.

If one wishes to improve the theoretical accuracy of this difference method, one may modify the order of accuracy of each operator more or less independently. In an earlier paper (Gerrity et al. 1972), we used such an approach for the integration of the shallow water equations with generally positive results.

To simply express the higher order, accurate, finite-difference operators, one should generalize the symbolic notation of eq (9) and (10). Only spatial variation will be considered since second-order accuracy in the time derivatives is sufficient for most meteorological problems. We define, with m an integer,

$$\overline{[f]}^{mx}=\tfrac{1}{2}[f_{j+m/2}^n+f_{j-m/2}^n] \tag{12}$$

and

$$[f]_{mx}=\frac{1}{m\Delta x}\,[f_{j+m/2}^n-f_{j-m/2}^n]. \tag{13}$$

One may again use Taylor series expansions to show that the following operators have fourth-order accuracy in Δx:

$$\overline{[f]}^{x_h}\equiv\tfrac{9}{8}\overline{[f]}^x-\tfrac{1}{8}\overline{[f]}^{3x} \tag{14}$$

and

$$[f]_{x_h}\equiv\tfrac{9}{8}[f]_x-\tfrac{1}{8}[f]_{3x} \tag{15}$$

where the subscript h is used to denote the higher order nature of the approximation. These operators may be combined with the second-order operators to produce the following eight, mixed forms for the approximation of the advection term in eq (1):

$$\overline{\overline{u}^x\psi_x}^x,\ \overline{\overline{u}^x\psi_x}^{x_h},$$
$$\overline{\overline{u}^x\psi_{x_h}}^x,\ \overline{\overline{u}^x\psi_{x_h}}^{x_h},$$
$$\overline{\overline{u}^{x_h}\psi_x}^x,\ \overline{\overline{u}^{x_h}\psi_x}^{x_h},$$

and

$$\overline{\overline{u}^{x_h}\psi_{x_h}}^x,\ \overline{\overline{u}^{x_h}\psi_{x_h}}^{x_h}. \tag{16}$$

In view of Crowley's success with the conservation form for the approximation of the advection equation, it is worthwhile noting that certain of the forms (expression 16) have conservation analogs, such as

$$\overline{\overline{u}^x\psi_x}^x=\overline{(u\psi)_x}^x-\overline{\overline{\psi}^x u_x}^x \tag{17a}$$

and

$$\overline{\overline{u}^x\psi_x}^{x_h}=\overline{(u\psi)_x}^{x_h}-\overline{\overline{\psi}^x u_x}^{x_h}, \tag{17b}$$

whereas precise conservation analogs probably do not exist for other forms; for example,

$$\overline{\overline{u}^x\psi_{x_h}}^x=\tfrac{9}{8}[\overline{(u\psi)_x}^x-\overline{\overline{\psi}^x u_x}^x]-\tfrac{1}{8}\overline{\overline{u}^x\psi_{3x}}^x. \tag{18}$$

One should also observe that the mixed higher order, accurate, approximations cannot be applied uniformly over the entire region of integration. As the boundaries are approached, one must switch to lower order schemes or introduce computational boundary conditions. In the study reported here, periodicity was assumed so that the higher order schemes were applicable over the entire spatial domain.

A principal alternative to the use of higher order, accurate, finite-difference schemes involves the use of a reduced size of the grid mesh, Δx, or Δt. In this study, we considered an integration based on a finer mesh version of eq (11). The space mesh, Δx, was reduced to one-half its value in other calculations. To maintain linear computational stability, we also reduced the time mesh, Δt, to one-half its value.

4. RESULTS

There are a considerable number of comparisons that might be made among the several solutions that were calculated. Since the problem studied may be easily replicated by other investigators, we shall confine our discussion to comparisons that are particularly suggestive.

In figure 1, we illustrate a deficiency of the formulation of the problem as a test for the significance of higher order, accurate, finite-difference approximations. This figure depicts the analytic solution (shown everywhere as curve T) and the two approximations,

$$\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_x}^x, \tag{19}$$

shown as curve A,

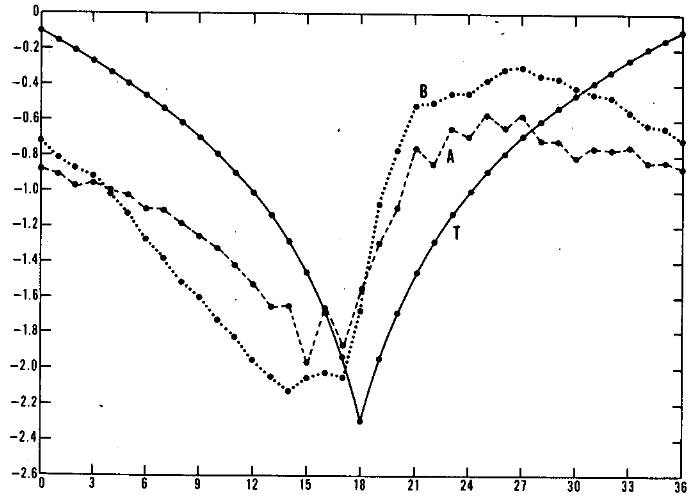

FIGURE 1.—Numerical solutions after 10 intervals of repetition. Curve A was calculated using $\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_x}^x$, curve B calculated using $\overline{\psi}^t_t=-\overline{\overline{u}^{x_h}\psi_{x_h}}^x$, and curve T is the analytic solution.

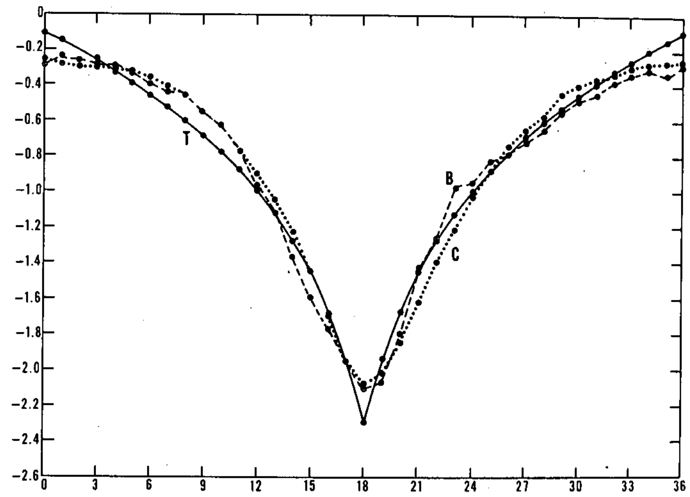

FIGURE 2.—Numerical solutions after 10 intervals of repetition. Curve B was calculated with $\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_x}^{x_h}$, curve C was interpolated from Crowley's figure showing the result of a fourth-order accurate conservation scheme, and curve T is the analytic solution.

and

$$\overline{\psi}^t_t=-\overline{\overline{u}^{x_h}\psi_{x_h}}^x, \tag{20}$$

shown as curve B.

This result is surprising, showing as it does a somewhat worse result when the higher order approximations were used. It is possible to account for this dilemma by observing that, at the singular points of the wind field, $\overline{u}^x$ yields a superior estimate of the wind in comparison to $\overline{u}^{x_h}$. The theoretical superiority of $\overline{u}^{x_h}$ depends upon the function having a relatively smooth variation. Except in the neighborhood of the singular points, the two approximations are identical. The situation is much the same with respect to the derivative of ψ. Initially, the derivative is discontinuous at two points and elsewhere slowly varying. Consequently, ψ_{x_h} is not everywhere more accurate than ψ_x as would be the case with a regular function.

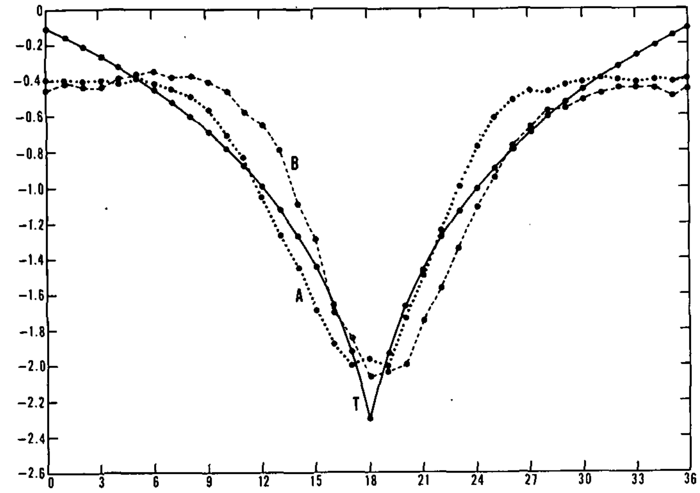

FIGURE 3.—Numerical solutions after 10 intervals of repetition. Curve A was calculated with fine mesh using $\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_x}^x$, curve B was calculated with regular mesh using $\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_{x_h}}^{x_h}$, and curve T is the analytic solution.

In figure 2, we show the result of

$$\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_x}^{x_h} \tag{21}$$

as curve B and Crowley's best result as curve C. In view of eq (17b), one may regard eq (21) as displaying a reasonable analog to the "conservation" property emphasized by Crowley. The equivalent fourth-order accuracy of eq (21) may be attributed to the redundant character of the semimomentum approximation's lattice structure, the preservation of equivalent fine-mesh accuracy by the interpolation operator, and the relatively "long-wave" structure of the advected field, ψ (cf. table 1).

It is our opinion that, in a more general case, one would find that the use of fourth-order estimates of the first derivative would be beneficial to the accuracy of the solution. It should be noted that the use of eq (21) required a reduction of the time step, so that

$$\frac{|u_{\max}|\Delta t}{\Delta x}\leq 0.72. \tag{22}$$

A somewhat larger value might be used, but instability was encountered when

$$\frac{|u_{\max}|\Delta t}{\Delta x}=0.9. \tag{23}$$

Little significance need be attached to this reduction in time step allowed by higher order advection estimates. The limit time step in meteorological prediction is associated with gravity waves, not with advective processes.

In figure 3, we present a final result. Curve A denotes the result obtained using eq. (19) on the fine mesh. Curve B shows the result obtained with the form,

$$\overline{\psi}^t_t=-\overline{\overline{u}^x\psi_{x_h}}^{x_h}. \tag{24}$$

The mean-square errors with these two methods are 0.0377 for eq (24); and 0.0274 for the fine-mesh calculation. The mean square error for eq (21), shown as curve B in figure 2, is 0.0094.

Comparison of curve A in figure 3 with curve A in figure 1 shows that a considerable improvement in accuracy was obtained by using a finer mesh. It is particularly noteworthy, however, that the results obtained with the higher order interpolation operator (curve B in figure 2) and by Crowley (curve C in figure 2) are both somewhat more accurate than the fine-mesh calculation.

5. CONCLUSIONS

The results obtained in this study substantiate the view that higher order approximations or finer mesh grids are equally valid methods for attaining greater accuracy in the numerical solution of meteorological equations. Of the two methods, the higher order scheme appears to be more efficient and accurate.

The simple approach employed to formulate higher order approximations based upon the semimomentum difference scheme gave excellent results, quite comparable to the conservation scheme used by Crowley. The analytic data used in the study were not sufficiently general to permit a satisfactory assessment of the full range of difference schemes. To accommodate evaluation of the performance of the higher order derivative, one might try to modify the form of the advected field.

Further study of the long-term computational stability of the higher order approximations should be conducted. Additionally, an evaluation of the requirement for computational boundary conditions for use with higher order schemes is required.

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